Wang Yong, Yuan Jun, Cao Duanlin*, Wang Jianlong and Chen Lizhen

The crystal structure of bis(4-nitroimidazole-1-yl) methane, $C_7H_6N_6O_4$

Table 1: Data collection and handling.

Crystal:	Block, colorless
Size:	$0.16 \times 0.11 \times 0.08$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.14 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, ω -scans
θ_{max} , completeness:	26.4° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	17779, 3885, 0.035
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3131
$N(\text{param})_{\text{refined}}$:	307
Programs:	Bruker programs [1], SHELX [2, 3], OLEX2 [4]

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Abstract

$C_7H_6N_6O_4$, monoclinic, $P2_1/c$ (no. 14), $a = 21.0402(7)$ Å, $b = 7.9959(3)$ Å, $c = 11.8012(4)$ Å, $\beta = 102.379(1)^\circ$, $V = 1939.22(12)$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0481$, $wR_{\text{ref}}(F^2) = 0.1296$, $T = 170$ K.

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The crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was prepared by nitrifying bis(imidazole-1-yl)methane. The title compound was recrystallized from ether solution at 293 K for 2 days to give colorless crystals.

***Corresponding author: Cao Duanlin**, School of Chemical Engineering and Technology, North University of China, Taiyuan 030051, Shanxi Province, P.R. China, e-mail: 575510418@qq.com
Wang Yong, Wang Jianlong and Chen Lizhen: School of Chemical Engineering and Technology, North University of China, Taiyuan 030051, Shanxi Province, P.R. China. <https://orcid.org/0000-0003-2992-9908> (W. Yong)

Yuan Jun: North University of China, Shuozhou, Shuozhou, 036000, Shanxi Province, P.R. China

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.51996(9)	0.0045(2)	0.74135(15)	0.0593(5)
O2	0.59384(8)	0.0466(2)	0.64212(16)	0.0595(5)
O3	0.37100(7)	0.8863(2)	0.72055(15)	0.0494(4)
O4	0.28112(8)	0.8320(2)	0.77591(14)	0.0457(4)
O5	0.76985(11)	−0.1984(2)	0.27015(16)	0.0682(6)
O6	0.86232(11)	−0.0747(3)	0.27101(17)	0.0706(6)
O7	0.98989(8)	−0.2980(2)	1.01603(15)	0.0494(4)
O8	0.89684(8)	−0.1999(2)	1.03517(14)	0.0473(4)
N1	0.53978(9)	0.0682(2)	0.66043(17)	0.0453(5)
N2	0.51421(9)	0.2598(2)	0.49720(17)	0.0438(4)
N3	0.40881(8)	0.2963(2)	0.48938(14)	0.0323(4)
N4	0.32062(8)	0.4694(2)	0.51962(15)	0.0349(4)
N5	0.25439(10)	0.5756(3)	0.6235(2)	0.0625(7)
N6	0.32105(8)	0.8039(2)	0.71549(15)	0.0369(4)
N7	0.81427(11)	−0.1034(3)	0.31257(17)	0.0515(5)
N8	0.76113(9)	−0.0429(2)	0.47366(16)	0.0421(4)
N9	0.83789(8)	0.1188(2)	0.57747(15)	0.0351(4)
N10	0.91305(7)	0.0930(2)	0.75936(14)	0.0338(4)
N11	0.99290(8)	−0.0799(2)	0.83821(15)	0.0356(4)
N12	0.94339(8)	−0.2031(2)	0.98760(15)	0.0365(4)
C1	0.43008(10)	0.1908(3)	0.57943(18)	0.0369(5)
H1	0.405367	0.141241	0.629143	0.044*
C2	0.49453(10)	0.1719(2)	0.58274(17)	0.0341(4)
C3	0.46082(10)	0.3334(3)	0.44252(19)	0.0404(5)
H3	0.458624	0.404637	0.377390	0.048*
C4	0.34333(10)	0.3527(3)	0.44190(18)	0.0387(5)
H4A	0.313802	0.254886	0.428093	0.046*
H4B	0.341946	0.407937	0.366354	0.046*
C5	0.35072(9)	0.6089(3)	0.57166(17)	0.0340(4)
H5	0.391383	0.654483	0.564595	0.041*

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
C6	0.30935(9)	0.6676(2)	0.63575(18)	0.0339(4)
C7	0.26291(12)	0.4567(3)	0.5516(3)	0.0635(8)
H7	0.231939	0.371163	0.525003	0.076*
C8	0.81183(11)	−0.0217(3)	0.42008(18)	0.0380(5)
C9	0.85972(10)	0.0763(3)	0.48104(18)	0.0386(5)
H9	0.899413	0.107965	0.460968	0.046*
C10	0.77865(10)	0.0445(3)	0.56942(19)	0.0394(5)
H10	0.753131	0.054811	0.626419	0.047*
C11	0.87474(10)	0.2089(3)	0.67704(19)	0.0394(5)
H11A	0.844517	0.271369	0.715254	0.047*
H11B	0.903965	0.290556	0.650992	0.047*
C12	0.89224(9)	0.0136(3)	0.84660(18)	0.0346(4)
H12	0.852026	0.027650	0.869765	0.042*
C13	0.94201(9)	−0.0905(2)	0.89307(17)	0.0319(4)
C14	0.97355(10)	0.0324(3)	0.75756(18)	0.0369(5)
H14	0.998665	0.067801	0.703964	0.044*

Experimental details

All H atoms were positioned geometrically and treated as riding, with N—H bond 0.88 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. Difference electron density peaks and holes near N1 suggest a small (not introduced) disorder at that group.

Discussion

Nitroimidazole derivatives is one of the research focuses on energetic materials [5, 6]. A series of compounds have been synthesized, such as 1,4-dinitroimidazole, 2,4-dinitroimidazole, 2,4,5-trinitroimidazole and 1-methyl-2,4,5-trinitroimidazole, etc. [7–10]. Nitroimidazole derivatives bridged by methylene are also expected to become a new energetic material, the title compound is one of them. Here we report the crystal structure of the title compound (*cf.* the figure).

The asymmetric unit of the title structure contains two crystallographically independent bis(4-Nitroimidazol-1yl)-methane molecules. The imidazole ring and nitro is almost flat.

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